NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS INTER General Internet Information NEWS LOGIN Welcome Banner and News Items

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NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 09:00:33 ON 29 APR 2004

=> FIL STNGUIDE

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION

0.21

0.21

FILE 'STNGUIDE' ENTERED AT 09:00:38 ON 29 APR 2004
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Apr 23, 2004 (20040423/UP).

=> FIL HOME

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION 0.06 0.27

FILE 'HOME' ENTERED AT 09:00:40 ON 29 APR 2004

=> file retg

FULL ESTIMATED COST

'RETG' IS NOT A VALID FILE NAME

SESSION CONTINUES IN FILE 'HOME'

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 0.21 0.48

FILE 'REGISTRY' ENTERED AT 09:01:18 ON 29 APR 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 27 APR 2004 HIGHEST RN 677274-15-6 DICTIONARY FILE UPDATES: 27 APR 2004 HIGHEST RN 677274-15-6

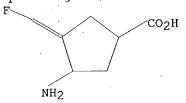
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

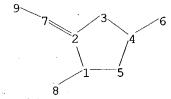
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> Uploading C:\Examination Auxillary files\10623152\10623152 clm 1.str



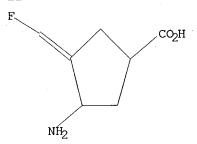


chain nodes:
6 7 8 9
ring nodes:
1 2 3 4 5
chain bonds:
1-8 2-7 4-6 7-9
ring bonds:
1-2 1-5 2-3 3-4 4-5
exact/norm bonds:
1-2 1-5 1-8 2-3 3-4 4-5
exact bonds:
2-7 4-6 7-9

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 11 exact full
FULL SEARCH INITIATED 09:02:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED

1 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L2

0 SEA EXA FUL L1

=>

Uploading C:\Examination Auxillary files\10623152\10623152 clm 1 obv X.str

9 7 3 6

chain nodes:
6 7 8 9
ring nodes:
1 2 3 4 5
chain bonds:

1-8 2-7 4-6 7-9

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-8 2-3 3-4 4-5

exact bonds: 2-7 4-6 7-9

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS

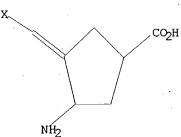
L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3

STR



Structure attributes must be viewed using STN Express query preparation.

=> search 13 sss full FULL SEARCH INITIATED 09:06:17 FILE 'REGISTRY' COMMAND INTERRUPTED

If this message appears repeatedly, please notify the Help Desk. Enter "HELP STN" for information on contacting the nearest STN Help Desk by telephone or via SEND in the STNMAIL file.

=> search 13 sss full
FULL SEARCH INITIATED 09:06:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

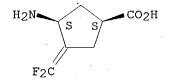
L4 1 SEA SSS FUL L3

=> d scan

L4 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

MF C7 H9 F2 N O2

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d 14

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 640897-20-7 REGISTRY

CN Cyclopentanecarboxylic acid, 3-amino-4-(difluoromethylene)-, (1S,3S)-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN (+)-(15,4S)-4-Amino-3-(difluoromethylene)-1-cyclopentanecarboxylic acid

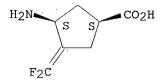
FS STEREOSEARCH

MF C7 H9 F2 N O2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (+).



- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL SESSION 213.22 213.70

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 09:07:08 ON 29 APR 2004
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FILE COVERS 1907 - 29 Apr 2004 VOL 140 ISS 18 FILE LAST UPDATED: 28 Apr 2004 (20040428/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 14

т 5

1 L4

=> d 15 ti fbib abs

- L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Design, Synthesis, and Biological Activity of a Difluoro-Substituted, Conformationally Rigid Vigabatrin Analogue as a Potent γ-Aminobutyric Acid Aminotransferase Inhibitor
- AN 2003:884657 CAPLUS
- DN 140:76841
- TI Design, Synthesis, and Biological Activity of a Difluoro-Substituted, Conformationally Rigid Vigabatrin Analogue as a Potent $\gamma\textsc{-Aminobutyric}$ Acid Aminotransferase Inhibitor
- AU Pan, Yue; Qiu, Jian; Silverman, Richard B.
- CS Department of Chemistry, Department of Biochemistry, Molecular Biology and Cell Biology and Drug Discovery Program, Northwestern University, Evanston, IL, 60208-3113, USA
- SO Journal of Medicinal Chemistry (2003), 46(25), 5292-5293 CODEN: JMCMAR; ISSN: 0022-2623
- PB American Chemical Society
- DT Journal
- LA English
- AB Previously it was found that a conformationally rigid analog [(1R,4S)-4-amino-2-cyclopentene-1-carboxylic acid] of the epilepsy drug (S)-vigabatrin did not inactivate γ-aminobutyric acid aminotransferase (GABA-AT). Ring opening of (1S,4S)-6-methylene-2-(phenylmethyl)-2-azabicyclo[2.2.1]heptan-3-one gave (1S,4S)-4-amino-3-methylene-1-cyclopentanecarboxylic acid (I). I, having an exocyclic

double bond, was found to inactivate GABA-AT, but only in the absence of 2-mercaptoethanol. The corresponding difluoro-substituted analog [(+)-(1S,4S)-4-amino-3-(difluoromethylene)-1-cyclopentanecarboxylic acid] was synthesized and was shown to be a very potent time-dependent inhibitor, even in the presence of 2-mercaptoethanol.

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	8.67	222.37
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY -0.69	SESSION -0.69

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 09:15:40 ON 29 APR 2004

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * * SESSION RESUMED IN FILE 'CAPLUS' AT 09:19:16 ON 29 APR 2004 FILE 'CAPLUS' ENTERED AT 09:19:16 ON 29 APR 2004 COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS FULL ESTIMATED COST	SINCE FILE ENTRY 8.67	TOTAL SESSION 222.37
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.69	0.69
=> file reg COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	9.11	222.81
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL
CA SUBSCRIBER PRICE	-0.69	-0.69

FILE 'REGISTRY' ENTERED AT 09:19:59 ON 29 APR 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 27 APR 2004 HIGHEST RN 677274-15-6 DICTIONARY FILE UPDATES: 27 APR 2004 HIGHEST RN 677274-15-6

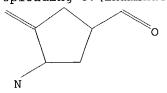
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> Uploading C:\Examination Auxillary files\10623152\10623152 clm 1 obv bare bones.str



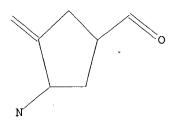
6 3 8 9 1 5 7

chain nodes:
6 7 8 9
ring nodes:
1 2 3 4 5
chain bonds:
1-7 2-6 4-8 8-9
ring bonds:
1-2 1-5 2-3 3-4 4-5
exact/norm bonds:
1-2 1-5 1-7 2-3 3-4 4-5 8-9
exact bonds:
2-6 4-8

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS

L6 STRUCTURE UPLOADED

=> d 16 L6 HAS NO ANSWERS L6 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 16 sss

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET: full FULL SEARCH INITIATED 09:20:40 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 4217 TO ITERATE

100.0% PROCESSED 4217 ITERATIONS SEARCH TIME: 00.00.01

15 ANSWERS

ь7

15 SEA SSS FUL L6

=> d scan

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1,1-Cyclopentanedicarboxylic acid, 3-methylene-4-[2-[(4methylphenyl)sulfonyl]hydrazino]-, diethyl ester (9CI)

MF C19 H26 N2 O6 S

$$\begin{array}{c|c} O & CH_2 \\ \parallel & \\ S-NH-NH \\ \hline \\ O & \\ EtO-C & \parallel \\ O & \\ O & \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1,1-Cyclopentanedicarboxylic acid, 3-[(4,5-dimethyl-1H-1,2,3-triazol-1-yl)amino]-4-[(phenylthio)methylene]-, diethyl ester, (E)- (9CI)

MF C22 H28 N4 O4 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

MF C12 H17 N O6

Relative stereochemistry.

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

MF C17 H19 N O6

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

MF C14 H19 N O6

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

MF C21 H32 N2 O9

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

MF C7 H9 F2 N O2

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1,1-Cyclopentanedicarboxylic acid, 4-methylene-3-[[(4methylphenyl)sulfonyl]amino]-2-phenyl-, dimethyl ester, trans- (9CI)

MF C23 H25 N O6 S

Relative stereochemistry.

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

1,1-Cyclopentanedicarboxylic acid, 3-[(4,5-dimethyl-1H-1,2,3-triazol-1-yl)amino]-4-[(phenylthio)methylene]-, diethyl ester, (Z)- (9CI)

MF C22 H28 N4 O4 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1,1-Cyclopentanedicarboxylic acid, 3-[(phenylmethoxy)amino]-4-[(phenylthio)methylene]-, diethyl ester, (Z)- (9CI)

MF C25 H29 N O5 S

Double bond geometry as shown.

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1,1-Cyclopentanedicarboxylic acid, 3-methyl-4-methylene-3-nitro-2-pentyl-, dimethyl ester, (2R,3S)-rel- (9CI)

MF C16 H25 N O6

Relative stereochemistry.

O OMe
$$R$$

$$(CH_2)_4$$

$$R$$

$$R$$

$$R$$

$$Me$$

$$Me$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):file caplus 'FILE CAPLUS' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END". HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN 1,1(2H)-Pentalenedicarboxylic acid, hexahydro-3-methylene-3a-nitro-, dimethyl ester, (3aR,6aS)-rel- (9CI)

MF C13 H17 N O6

Relative stereochemistry.

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

1,1-Cyclopentanedicarboxylic acid, 2-(2,2-dimethyl-1,3-dioxolan-4-yl)-3methyl-4-methylene-3-nitro-, dimethyl ester, (2R,3R)-rel- (9CI)

MF C16 H23 N O8

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Cyclopentanecarboxylic acid, 3-amino-4-methylene-, (1S,3S)- (9CI)

MF C7 H11 N O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

MF C19 H25 N O5

$$\begin{array}{c} \text{O} \\ \parallel \\ \text{C-OEt} \\ \text{Ph-CH}_2\text{-O-NH} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION 156.68 379.49 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION -0.69 0.00 CA SUBSCRIBER PRICE

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FILE COVERS 1907 - 29 Apr 2004 VOL 140 ISS 18 FILE LAST UPDATED: 28 Apr 2004 (20040428/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 17

 $\Gamma8$

6 L7

=> aminotransferase

25565 AMINOTRANSFERASE 6096 AMINOTRANSFERASES

L9 27732 AMINOTRANSFERASE

(AMINOTRANSFERASE OR AMINOTRANSFERASES)

=> 18 and 19 L10 1 L8 AND L9

=> d 110

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:884657 CAPLUS

DN 140:76841

TI Design, Synthesis, and Biological Activity of a Difluoro-Substituted, Conformationally Rigid Vigabatrin Analogue as a Potent γ-Aminobutyric Acid Aminotransferase Inhibitor

AU Pan, Yue; Qiu, Jian; Silverman, Richard B.

CS Department of Chemistry, Department of Biochemistry, Molecular Biology and Cell Biology and Drug Discovery Program, Northwestern University, Evanston, IL, 60208-3113, USA

SO Journal of Medicinal Chemistry (2003), 46(25), 5292-5293 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION 383.68 FULL ESTIMATED COST 4.19 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION 0.00 -0.69CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 09:23:48 ON 29 APR 2004

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

Web Page URLs for STN Seminar Schedule - N. America NEWS "Ask CAS" for self-help around the clock NEWS Source of Registration (SR) information in REGISTRY updated NEWS JAN 27 and searchable A new search aid, the Company Name Thesaurus, available in NEWS JAN 27 CA/CAplus German (DE) application and patent publication number format NEWS 5 FEB 05 changes

NEWS 6 MAR 03 MEDLINE and LMEDLINE reloaded

NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded

NEWS 8 MAR 03 FRANCEPAT now available on STN

NEWS	9	MAR	Pharmaceutical Substances (PS) now available on STN	
NEWS	10	MAR	WPIFV now available on STN	
NEWS	11	MAR	No connect hour charges in WPIFV until May 1, 2004	
NEWS	12	MAR	New monthly current-awareness alert (SDI) frequency in	RAPRA
NEWS	13	APR	PROMT: New display field available	
NEWS	14	APR	FIPAT/IFIUDB/IFICDB: New super search and display fiel	d
			available	
NEWS	15	APR	LITALERT now available on STN	
NEWS	16	APR	NLDB: New search and display fields available	
			,	
NEWS	EXP	RESS	ARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT	
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),				
			ND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004	
NEWS	HOU	RS	TN Operating Hours Plus Help Desk Availability	
NEWS	INT	ER	eneral Internet Information	
NEWS	LOG	IN	elcome Banner and News Items	
NEWS	PHO	NE	irect Dial and Telecommunication Network Access to STN	
NEWS	WWW		AS World Wide Web Site (general information)	

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * STN Columbus *

FILE 'HOME' ENTERED AT 10:43:22 ON 29 APR 2004

=> ogoff

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS

SINCE FILE ENTRY SESSION 0.21

TOTAL

0.21

FULL ESTIMATED COST

STN INTERNATIONAL LOGOFF AT 10:43:43 ON 29 APR 2004